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Modular Invariance of Finite Size Corrections and a Vortex Critical Phase.

by

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Abstract: We analyze a continuous spin Gaussian model on a toroidal triangular lattice with periods L_0 and L_1 where the spins carry a representation of the fundamental group of the torus labeled by phases u_0 and u_1 . We find the *exact finite size and lattice corrections*, to the partition function Z , for arbitrary mass m and phases u_i . Summing $Z^{-1/2}$ over phases gives the corresponding result for the Ising model. The limits $m \rightarrow 0$ and $u_i \rightarrow 0$ do not commute. With $m = 0$ the model exhibits a *vortex critical phase* when at least one of the u_i is non-zero. In the continuum or scaling limit, for arbitrary m , the finite size corrections to $-\ln Z$ are *modular invariant* and for the critical phase are given by elliptic theta functions. In the cylinder limit $L_1 \rightarrow \infty$ the “cylinder charge” $c(u_0, m^2 L_0^2)$ is a non-monotonic function of m that ranges from $2(1 + 6u_0(u_0 - 1))$ for $m = 0$ to zero for $m \rightarrow \infty$.

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Finite size effects are an intrinsic feature of laboratory experiments which probe the neighbourhood of a continuous phase transition. The scaling properties of these corrections to the infinite (bulk) system behaviour play an increasingly important role in computer simulations and our theoretical understanding of the critical regime of statistical systems [1]. The interplay of these effects with other aspects of the system can give rise to crossover from one characteristic behaviour to another [2]. It is possible to make real progress in the detailed analysis of such situations in two dimensions and for this reason two dimensional models have attracted much interest in recent years. Many of their properties are expressible in terms of those of generalized Gaussian models [3] and with minor modification the results of this note can be adapted to a wide class of other models.

Pure finite size effects can be isolated from those due to the presence of a boundary by ensuring that the connectivity of the underlying lattice is such that it has no boundary. One can avoid other complications, such as local curvature of the lattice, while retaining the finite size effects, by considering a *flat torus*. Furthermore, in two dimensions, the *only* zero curvature finite volume manifold without boundary is the *flat torus*. This torus can be conveniently thought of as a parallelogram with opposite sides identified. We take the sides to be of length L_0 and L_1 , with L_0 at an angle θ to L_1 , cf. fig. 1. Simple geometry then means that the point (x, y) is thereby identified with the point $(x + aL_1 \cos \theta + bL_0, y + aL_1 \sin \theta)$ where a and b are integers.

We consider a triangular lattice composed of similar triangles, pairs of which form parallelograms, cf. fig. 1. The basic triangles have two sides of lengths a_0 and a_1 with an angle θ between them. The complete lattice forms our torus, T^2 , and consists of $K_0 K_1$ sites and $2K_0 K_1$ triangles, forming a parallelogram of sides $L_0 = K_0 a_0$ and $L_1 = K_1 a_1$.

We take a complex continuous spin variable $\varphi(x, y)$ on T^2 but will *not* demand that φ be periodic, though the underlying lattice is, rather it acquires a phase on being transported

around one of the cycles of the torus. In general we require that

$$\varphi(x + aL_1 \cos \theta + bL_0, y + aL_1 \sin \theta) = e^{2\pi i(au_1 + bu_0)} \varphi(x, y), \quad a, b \in \mathbf{Z} \quad (1)$$

For u_0 and u_1 neither integer or half integer the spin variable is necessarily either complex or real with two components: From the two component viewpoint these boundary conditions can be thought of as corresponding to vortices winding around the periods of the torus. From a mathematical standpoint φ is a section of a bundle \mathcal{L} over the torus T^2 .

Labeling the lattice sites by $(k_0, k_1) \equiv \mathbf{k} = k_0 + (k_1 - 1)K_0$ with $k_i = 1, \dots, K_i$, the energy of a configuration is given by

$$\mathcal{E}_{\mathcal{L}}[T^2, \varphi^*, \varphi] = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} \sqrt{g} \varphi^*(\mathbf{k}) \left(\Delta(\mathbf{k}, \mathbf{k}') + m^2 \delta_{\mathbf{k}, \mathbf{k}'} \right) \varphi(\mathbf{k}') \quad (2)$$

where $\sqrt{g} = a_0 a_1 \sin \theta$ and $\delta_{\mathbf{k}, \mathbf{k}'}$ is the Kronecker delta. Δ is a $K_0 K_1 \times K_0 K_1$ *symmetric* matrix, all entries of which are determined by nearest neighbour interactions, so that each spin interacts with six neighbouring spins. Explicitly the only non-zero elements are those given below (and their transposes): we have

$$\begin{aligned} \Delta\{(k_0, k_1), (k_0 + 1, k_1)\} &= -\alpha = -\frac{1}{\sin^2 \theta} \left(\frac{1}{a_0^2} - \frac{\cos \theta}{a_0 a_1} \right) \\ \Delta\{(k_0, k_1), (k_0, k_1 + 1)\} &= -\beta = -\frac{1}{\sin^2 \theta} \left(\frac{1}{a_1^2} - \frac{\cos \theta}{a_0 a_1} \right) \\ \Delta\{(k_0 + 1, k_1), (k_0, k_1 + 1)\} &= -\gamma = -\frac{1}{\sin^2 \theta} \left(\frac{\cos \theta}{a_0 a_1} \right) \\ \Delta\{(k_0, k_1), (k_0, k_1)\} &= 2\sigma, \quad \text{where } \sigma = \alpha + \beta + \gamma \end{aligned} \quad (3)$$

We actually solve the model for general nearest neighbour couplings, α , β and γ , in which case $g = (\alpha\beta + \beta\gamma + \gamma\alpha)^{-1}$. Despite the simplicity of the model we will see that it has a surprisingly rich structure.

The eigenfunctions of Δ that satisfy (1) are the discrete Fourier basis

$$e_{mn}(k_0, k_1) = \frac{1}{\sqrt{K_0 K_1}} \exp \left[2\pi i \left\{ (m + u_0) \frac{k_0}{K_0} + (n + u_1) \frac{k_1}{K_1} \right\} \right], \quad \text{with } \begin{cases} m = 1, \dots, K_0 \\ n = 1, \dots, K_1 \end{cases} \quad (4)$$

orthogonality of which is given by

$$\sum_{k_0=1}^{K_0} \sum_{k_1=1}^{K_1} e_{mn}^*(k_0, k_1) e_{m'n'}(k_0, k_1) = \delta_{m,m'} \delta_{n,n'} \quad (5)$$

while the corresponding sum over m and n gives completeness. The eigenvalues $\lambda_{n_0 n_1}$ of the matrix $\frac{1}{2}(\Delta + m^2)$ are then

$$\lambda_{n_0 n_1} = \delta - \alpha \cos(x_{n_0}) - \beta \cos(x_{n_1}) - \gamma \cos(x_{n_0} - x_{n_1})$$

where $x_{n_i} = \frac{2\pi(n_i + u_i)}{K_i}$, $i = 0, 1$ and $\delta = \sigma + \frac{m^2}{2}$ (6)

We are interested in the partition function

$$Z(T^2, \mathcal{L}, m) = \int \left[\prod d\varphi^* d\varphi \right] e^{-\frac{1}{k_B T} \mathcal{E}_{\mathcal{L}}[T^2, \varphi^*, \varphi]} = \prod_{(n_0, n_1)}^{(K_0, K_1)} \left\{ \frac{\pi k_B T}{\sqrt{g} \lambda_{n_0 n_1}} \right\} \quad (7)$$

The free energy is then given by $F = k_B T W$ where $W = -\ln Z$.

To perform the sums we note the rearrangement of the eigenvalues

$$\lambda_{n_0 n_1} = \delta - \alpha \cos x_{n_0} - |\beta_{n_0}| \cos(x_{n_1} - \theta_{n_0}) \quad \text{where} \quad \beta_{n_0} = \beta + \gamma e^{ix_{n_0}} = |\beta_{n_0}| e^{i\theta_{n_0}} \quad (8)$$

and use the basic non-trivial identity [4]

$$\sum_{n=0}^{K-1} \ln[z - \cos x_n] = K \int_0^{\frac{\pi}{2}} \frac{d\nu}{\pi} \ln[z^2 - \cos^2 \nu] + \ln \left| 1 - \left(z - \sqrt{z^2 - 1} \right)^K e^{2\pi i u} \right|^2 \quad (9)$$

where $z \geq 1$ and real. In any case the sum over n_1 followed by that over n_0 yields:

$$W = K_0 K_1 W_B + W_F \quad (10)$$

where

$$W_B = \int_{-\pi}^{\pi} \frac{d\nu_1}{2\pi} \int_{-\pi}^{\pi} \frac{d\nu_2}{2\pi} \ln \left[\frac{\sqrt{g}}{\pi k_B T} \{ \delta - \alpha \cos(\nu_1) - \beta \cos(\nu_2) - \gamma \cos(\nu_1 - \nu_2) \} \right] \quad (11)$$

and

$$\begin{aligned}
W_F = K_1 \sum_{\epsilon=\pm} \int_0^{\frac{\pi}{2}} \frac{d\nu}{\pi} \ln \left| 1 - \left(q_\epsilon - \sqrt{q_\epsilon^2 - 1} \right)^{K_0} e^{2\pi i u_0} \right|^2 \\
+ \sum_{n_0=-\left[\frac{K_0}{2}\right]}^{\left[\frac{K_0-1}{2}\right]} \ln \left| 1 - e^{-K_1 v_{n_0}} e^{2\pi i u_1} \right|^2
\end{aligned} \tag{12}$$

here $[x]$ denotes the integer part of x . The definitions of the various variables in (12) above are as follows:

$$q_{\pm} = q \pm \sqrt{q^2 - p} \quad q = \frac{\alpha\delta + \beta\gamma \cos^2 \nu}{\alpha^2}, \quad p = \frac{\delta^2 - (\beta^2 + \gamma^2) \cos^2 \nu}{\alpha^2} \tag{13}$$

and

$$v_{n_0} = -\ln \left[z_{n_0} - \sqrt{z_{n_0}^2 - 1} \right] + i\theta_{n_0}, \quad \text{where} \quad z_{n_0} = \frac{\delta - \alpha \cos x_{n_0}}{2|\beta_{n_0}|} \tag{14}$$

Note that W_B gives the free energy per lattice site in the thermodynamic limit, i.e.

$$\lim_{K_0, K_1 \rightarrow \infty} \frac{W}{K_0 K_1} = W_B \tag{15}$$

hence, due to the fact that we are dealing with a finite rather than an infinite lattice, W_F gives the *complete finite size correction* to the bulk lattice behaviour.

If instead we perform the sum over n_0 before that over n_1 we find the alternative composition $W = K_0 K_1 W_B + \tilde{W}_F$. The two apparently different expressions W_F and \tilde{W}_F are, obviously, equal; they can be transformed into one another by the interchange of α with β and the subscripts 0 and 1.

The limit of interest to us is the *continuum* or *scaling* limit. This is a constrained thermodynamic limit achieved by taking $K_0, K_1 \rightarrow \infty$ while keeping fixed $L_i = K_i a_i$, θ , m^2 and the ratio $k = \frac{K_1}{K_0}$. The asymptotic form of W_B in this scaling limit is given by

$$W_B K_0 K_1 = K_0 K_1 \Lambda_B - \frac{V m^2}{4\pi} \{ \ln[K_0 K_1] - 2\rho \} - \frac{V m^2}{4\pi} (\ln[\frac{m^2 V}{4\pi^2}] - 1) + \dots \tag{16}$$

Here Λ_B is the value of W_B at $m = 0$ and

$$\rho \equiv \rho(\alpha, \beta, \gamma) = \int_0^\pi d\nu \left[\frac{1}{\sin \nu \sqrt{1 + g\alpha^2 \sin^2 \nu}} - \frac{1}{\nu} \right] - \frac{1}{2} \ln [\sqrt{g}(\beta + \gamma)] \quad (17)$$

Despite its appearance, $\rho(\alpha, \beta, \gamma)$ is *symmetric* under interchange of α and β . Both Λ_B and ρ depend on L_0 , L_1 , θ and k , or equivalently they depend on the geometry of the lattice triangle.

We find the limiting behaviour of W_F is given by^(a)

$$\Gamma_F = -\frac{\pi\tau_1}{6}c(u_0, \frac{m^2V}{\tau_1}) + \sum_{n=-\infty}^{\infty} \ln \left| 1 - e^{-2\pi\tau_1 \sqrt{(n+u_0)^2 + \frac{m^2V}{4\pi^2\tau_1}} + 2\pi i \{u_1 - \tau_0(n+u_0)\}} \right|^2 \quad (18)$$

where

$$\tau_0 = \frac{k}{\sqrt{g}|\beta + \gamma|}, \quad \tau_1 = \frac{k\gamma}{\beta + \gamma} \quad \text{and} \quad V = K_0 K_1 \sqrt{g} \quad (19)$$

The function $c(u, x)$ that appears in (18) is given by

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi} \ln \left| 1 - e^{-\sqrt{p^2 + x} + 2\pi i u} \right|^2 = -\frac{c(u, x)\pi}{6} \quad (20)$$

Corrections to (18) which vanish in the limit are also easily obtainable from (12). In terms of the torus geometry described above we have $\tau_0 = \frac{L_1}{L_0} \cos \theta$, $\tau_1 = \frac{L_1}{L_0} \sin \theta$ and $V = L_0 L_1 \sin \theta$.

Certain special cases of (18) arise in the case of an Ising model on a torus (see [5] where the case $\tau_0 = 0$ was studied). This can be understood from the equivalence of the Ising model to a dimer model on a decorated lattice where similar determinants arise [6]. From this equivalence, exhibiting the phase dependence of W_F by $W_F(u_0, u_1)$, with α , β , γ and δ obtained from [7], we have

$$Z^{Ising} = \frac{1}{2} e^{-W_B^{Ising}} \left\{ \mp e^{\frac{1}{2}W_F(0,0)} + e^{\frac{1}{2}W_F(0,\frac{1}{2})} + e^{\frac{1}{2}W_F(\frac{1}{2},0)} + e^{\frac{1}{2}W_F(\frac{1}{2},\frac{1}{2})} \right\} \quad (21)$$

(a) In extracting the limit, the expansions $\ln q_- = -\frac{\sqrt{g}}{2}(\beta + \gamma)^2(\nu^2 + \frac{gm^2}{\beta + \gamma}) + \dots$ and $v_{n_0} = \sqrt{\frac{1}{g(\beta + \gamma)|\beta + \gamma|}}x_{n_0}^2 + \frac{m^2}{|\beta + \gamma|} + i\frac{\gamma}{\beta + \gamma}x_{n_0} + \dots$ for small ν and m^2 are useful.

for ferromagnetic couplings, with $+$ referring to $T < T_c$ and $-$ to $T > T_c$. In the scaling limit $W_F \rightarrow \Gamma_F$. Our results therefore incorporate the complete lattice and finite size corrections for the Ising model on a triangular lattice. With a similar equivalence our results can easily be translated to give the general result for other models.

Γ_F is *invariant* under the transformations

$$\begin{aligned} \text{(i)} \quad & u_0 \mapsto u_0 & u_1 \mapsto u_0 + u_1 & \tau_0 \mapsto \tau_0 + 1 & \tau_1 \mapsto \tau_1 \\ \text{(ii)} \quad & u_0 \mapsto u_1 & u_1 \mapsto -u_0 & \tau_0 \mapsto -\frac{\tau_0}{|\tau|^2} & \tau_1 \mapsto \frac{\tau_1}{|\tau|^2} \end{aligned}$$

where $\tau = \tau_0 + i\tau_1$. Invariance under (i) is obvious from (18) and records the action of the generator ‘ T ’ of $SL(2, \mathbf{Z})/\mathbf{Z}_2$ while (ii) interchanges Γ_F with $\tilde{\Gamma}_F$ this latter being obtained by performing the sums leading to Γ_F in the opposite order. These two expressions are *equal* and (ii) records the action of the generator ‘ S ’ of the modular group $SL(2, \mathbf{Z})/\mathbf{Z}_2$. The volume V is invariant under the action these generators. But S and T generate the whole modular group $SL(2, \mathbf{Z})/\mathbf{Z}_2$ and so Γ_F and V are invariant under the action of any element of $SL(2, \mathbf{Z})/\mathbf{Z}_2$. Hence we can conclude that *in the scaling limit the complete finite size corrections to the bulk free energy are invariant under the entire modular group*.

If M denotes an arbitrary element of the modular group, under which τ undergoes the well known transformation $\tau \mapsto (a\tau + b)/(c\tau + d)$, we have that Γ_F is invariant under the replacement

$$\begin{aligned} u_1 \mapsto u_1[M] &= au_1 + bu_0 & u_0 \mapsto u_0[M] &= cu_1 + du_0 \\ L_1 \mapsto L_1[M] &= aL_1 + bL_0e^{-i\theta} & L_0 \mapsto L_0[M] &= cL_1e^{i\theta} + dL_0 \end{aligned} \tag{22}$$

where

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2, \mathbf{Z})/\mathbf{Z}_2, \quad a, b, c, d \in \mathbf{Z}, \quad ab - cd = 1 \tag{23}$$

We note that the sum over the four terms in (21) gives the finite size correction Z_F^{Ising} as a modular invariant function of τ_0 , τ_1 and m^2V . It is clear from our construction that summing over the phases u_i which form an orbit of $SL(2, \mathbf{Z})/\mathbf{Z}_2$ on the space of phases

(the Picard Variety [8]) will allow one to construct similar phase independent modular invariant partition functions, such as arise in other conformal field theories cf. [9] and references therein.

Taking $m \rightarrow 0$ in (18) we find the critical phase limit of Γ_F is given by

$$\begin{aligned}\Gamma_F &= -\frac{\pi\tau_1}{6}c(u_0) + \sum_{n=-\infty}^{\infty} \ln \left| 1 - e^{2\pi i\{\tau|n| - \epsilon_n(u_1 - \tau u_0)\}} \right|^2, \quad \epsilon_n = \frac{n + u_0}{|n + u_0|} \\ &= \ln \left| \frac{e^{\pi i u_0^2 \tau} \vartheta_1(u_1 - \tau u_0 | \tau)}{\eta(\tau)} \right|^2\end{aligned}\tag{24}$$

where $c(u) = 2\{1 - 6u(1 - u)\}$, ϑ_1 is a Jacobi theta function and η is the Dedekind eta function—the modular transformation properties of ϑ_1 and η are well known and allow an independent check of the modular invariance in this limit.

A further limit of interest is the geometric one obtained by taking $L_1 \rightarrow \infty$; it corresponds to a cylindrical geometry. In this limit Γ_F/V reduces to the expression $\gamma^{cylinder}$ where

$$\gamma^{cylinder} = -\frac{\pi}{6L_0^2}c(u_0, m^2 L_0^2)\tag{25}$$

(The analogous limit, where $L_0 \rightarrow \infty$, replaces u_0 and L_0 by u_1 and L_1 respectively.) When u_0 and m are both zero the “cylinder charge” $c(u_0, m^2 L_0^2)$ reduces to the central charge of the model; in our case $c = 2$. The cylinder charge should not be confused with the Zamolodchikov c -function [10] for this model, the two functions have different dependencies on m , the latter for example being a monotonic function of m . We plot $c(u, x)$ in fig. 2 for different values of u as a function of x . It exhibits the crossover to $c = 0$ at large values of x , and is clearly *not* a monotonic function of x . From (21) we see that

$$\gamma_{Ising}^{cylinder} = \frac{\pi}{12L_0^2}c\left(\frac{1}{2}, x\right)\tag{26}$$

Comparison with (25) means that the cylinder charge for the Ising model is $-\frac{1}{2}c(\frac{1}{2}, x)$, which for $x = 0$ gives the usual central charge $c = \frac{1}{2}$ [11].

The limits $m \rightarrow 0$ and $u_0, u_1 \rightarrow 0$ for Γ_F do not commute. To see this we expand Γ_F (18) for small m and u_0, u_1 obtaining

$$\Gamma_F = \ln \left[(2\pi)^2 |u_1 - \tau u_0|^2 + \tau_1 m^2 V \right] + 2 \ln |\eta(\tau)|^2 + \dots \quad (27)$$

and this expression clearly can tend to the distinct logarithmically singular expressions $\ln |u_1 - \tau u_0|^2 + 2 \ln |\eta(\tau)|^2$ and $\ln[\tau_1 m^2 V] + 2 \ln |\eta(\tau)|^2$ depending on the order in which the limits are taken. However both limits and indeed (27) itself are *modular invariant*.

The continuum version of the model studied here is described by the Hamiltonian

$$I[\varphi, L_0, L_1, \theta] = \frac{1}{2} \int_{T^2} \sqrt{g} \left[\partial_\mu \varphi^* g^{\mu\nu} \partial_\nu \varphi + m^2 \varphi^* \varphi \right] \quad (28)$$

It is a simple task to obtain the corresponding continuum partition function by the method of ζ -function regularisation. This procedure yields the finite size contribution Γ_f of (18) but the bulk term differs significantly being now $-\frac{Vm^2}{4\pi}(\ln[(m/2\pi\mu)^2] - 1)$ where μ is an arbitrary undetermined scale. Analogues of this continuum model were discussed in [9] where the phases were taken to be rational numbers. Their expressions unfortunately contain errors and they did not succeed in separating the bulk and finite size contributions.

The model we have studied above serves as a useful starting point for a perturbative treatment of the approach to the Kosterlitz-Thouless phase [12] in a $|\varphi|^4$ theory and thus captures the neighbourhood of the critical point of the XY model as the critical point is approached from the disordered phase. That the boundary conditions capture the essential features of a vortex phase can be seen by considering (1) in the cylinder limit and mapping the cylinder to the plane using the conformal map $y + i\frac{2\pi x}{L_0} = \ln z$. The charge of the vortex at the origin is then given by u_0 and its existence gives rise to an Aharonov-Bohm effect for transport around the origin.

In summary, the finite size corrections to the free energy are *modular invariant*. This conclusion extends to the entire scaling neighborhood of the critical phase. We use our

results to give expressions for the complete lattice and finite size corrections for the two dimensional Ising model on a triangular lattice via its equivalence to a sum over Pfaffians. Modular invariance also extends to models in more than two dimensions when the geometry giving rise to finite size effects contains a flat torus. For a three dimensional cylindrical geometry with toroidal cross-section the result can be obtained from Γ_f by replacing m^2 with $m^2 + q^2$ and integrating the resulting expression over q . One can understand the origin of modular invariance in general as the residual freedom to reparametrize coordinates, in the continuum limit, while retaining flat toroidal geometry.

In the two dimensional case the limiting finite size corrections at the critical phase are expressible in terms of classical elliptic functions. Infinitesimally small values of the phases u_i lead to logarithmically divergent contributions to the free energy. This implies that the free energy needed to create a vortex becomes infinite for an infinitely large lattice. In general the model has a surprisingly rich structure of non-commuting limits. For example the limits of approaching the critical phase and that of sending the u_i to zero do not commute.

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The triangulated torus

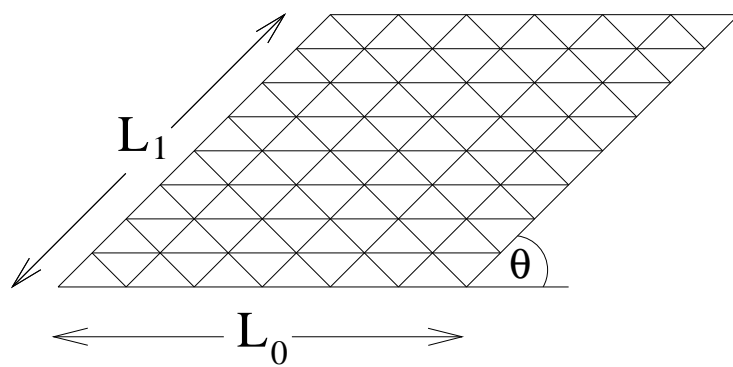


Fig. 1.

The ‘cylinder charge’ function $c(u, x)$ for various u

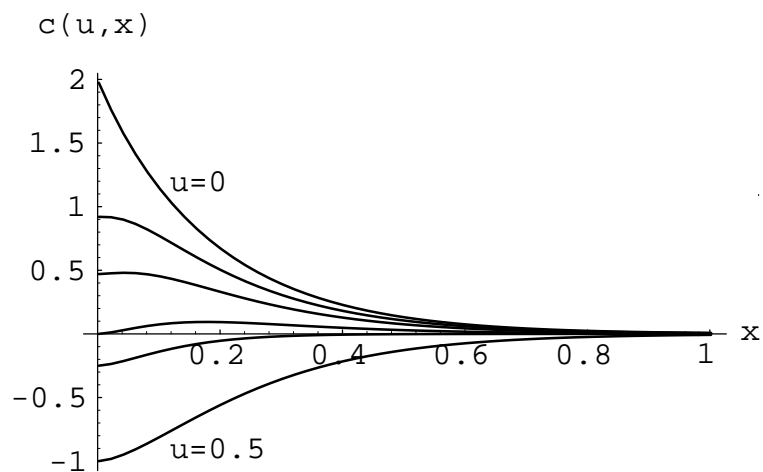


Fig. 2.

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